

Indian Institute of Space Science and Technology



Thiruvananthapuram

M.Tech. Materials Science and Technology
Curriculum and Syllabus
(Effective from 2024 Admission)

Department of Chemistry



Program Educational Objectives (PEO)

1. To provide foundational knowledge of key concepts in material science, including the properties, structures, and behaviors of various materials.
2. To equip the graduates to apply principles of material science to solve engineering problems and design new materials with desired properties.
3. To train the students to analyze material behavior and evaluate the impact of materials under different and environmental conditions.
4. To promote the students to integrate knowledge from different areas of material science to innovate and develop new materials and technologies.
5. To develop students' ability to critically assess the performance of materials in various applications and make decisions on material selection and optimization.

Program Outcomes (PO)

1. Graduates will have a comprehensive understanding of fundamental principles and advanced concepts in material science, including the structure-property relationships of materials.
2. Graduates will demonstrate advanced skills in material synthesis, processing, and characterization in various applications.
3. Graduates will analyze and interpret data from material characterization experiments, identifying trends and drawing meaningful conclusions.
4. Graduates will integrate knowledge from different areas of material science to design and develop new materials and innovative technologies.
5. Graduates will critically assess the suitability of materials for specific applications, considering factors like performance, cost, and environmental impact.
6. Graduates will exemplify integrity, ethical responsibility, and commitment to lifelong learning in their professional conduct.

M. Tech.

Materials Science and Technology



Chemistry

Curriculum and Course Content

(Syllabus revised: July 2024)

Eligibility Criteria

- **M.Sc. or M.S.** in Chemistry (all branches)/Physics/Materials Science/Nanoscience and Technology (GATE papers: CY/PH /XE)
- **B.Tech or B.E.** or equivalent degree in Polymer Science and Technology/Chemical Engineering/Rubber Technology/Plastic Technology/Metallurgy and Materials Science/ Mechanical Engineering/ Production and Industrial Engineering/Physical Sciences/ Chemical Technology/ Petrochemical Technology (GATE papers: CH/ XE/ MT/ ME)

Intake

- **12+1* students per year (*EWS)**

Course Structure

SEMESTER I	4 Core + 2 Elective + 2 Lab	20 credits
SEMESTER II	3 Core + 3 Elective + 2 Lab	20 credits
SEMESTER III	Project Phase I Seminar Summer internship	13 credits
SEMESTER IV	Project Phase II Comprehensive Viva	18 credits

Total 71 credits

Courses

Semester I

Code	Course Name	L-T-P	Credit
CHM611	Fundamentals of Materials Science	3-0-0	3
CHM612	Applied Mathematics and Process Modeling	3 0 0	3
CHM614	Materials Characterisation Techniques	3-0-0	3
CHM615	Nanoscience and Technology	3-0-0	3
CHM8xx	<i>Elective 1</i>	3-0-0	3
CHM8xx	<i>Elective 2</i>	3-0-0	3
CHM631	Lab 1: Applied Mathematics and Process Modeling	0-0-3	1
CHM633	Lab 2: Materials Synthesis and Characterization	0-0-3	1
	<i>Total credits in Sem I</i>		20

Semester II

Code	Course Name	L-T-P	Credit
CHM621	Processing and Design of Materials	3-0-0	3
CHM623	Composites Science and Technology	3-0-0	3
CHM624	Aerospace Materials	3-0-0	3
CHM8xx	<i>Elective 3</i>	3-0-0	3
CHM8xx	<i>Elective 4</i>	3-0-0	3
CHM8xx	<i>Elective 5</i>	3-0-0	3
CHM641	Lab 3: Composite and Processing	0-0-3	1
CHM644	Lab 4: Aerospace Materials	0-0-3	1
	<i>Total credits in Sem II</i>		20

Semester III

Code	Course Name	L-T-P	Credit
CHM851	Project I(Literature Survey, Presentations, Phase I of experimental work)		10
CHM854	Summer Internship		2
CHM855	Seminar		1
	<i>Total credits in Sem III</i>		13

Semester IV

Code	Course Name	L-T-P	Credit
CHM852	Project II(Phase II of experimental work, Data analysis and Dissertation, Viva-voce)		16
CHM853	Comprehensive viva		2
	<i>Total credits in Sem IV</i>		18
	Total credits		71

Semester	I	II	III	IV	Total
Credits	20	20	13	18	71

List of Electives

S.No.	Code	Course Name
1.	CHM864	Chemical Rocket Propellants
2.	CHM865	Thin Films and Surface Engineering
3.	CHM866	Mechanical Behavior of Materials
4.	CHM867	Paints and Coatings
5.	CHM868	Advanced Characterization Techniques
6.	CHM869	Corrosion Science and Technology
7.	CHM870	Thermodynamics And Phase Transformations in Materials
8.	CHM872	Fundamentals of Polymer Science
9.	CHM873	Specialty Polymers
10.	CHM874	Rubber Technology
11.	CHM875	Smart and Intelligent Materials
12.	CHM876	Membrane Separation Technology
13.	CHM877	Electrochemical Energy Storage systems
14.	CHM878	Materials for Renewable Energy Conversion

Revised Syllabus (July 2024)

CHM611

Fundamentals of Materials Science

Course Description:

This course focuses on the fundamental aspects of materials science which every material scientist is supposed to be familiar with. The course discusses the basic structure of solids, classification of materials based on the structure and the correlation between the structure and properties. The evolution of properties based on the structure and its alteration is also dealt with.

Course Objectives:

- To provide the students with basic knowledge of materials science, so that they would be able to understand and distinguish between variety of materials based on their structure and properties

Course Outcomes:

- Students will analyze and classify the different classes of materials used in engineering applications, and evaluate and justify the selection of appropriate materials for specific applications

Syllabus:

Structure of solids, Significance of structure property relationship; Diffusion phenomenon, Applications of diffusion; Principles of solidification, Phase diagrams and phase transformations, Heat treatment; Ceramic materials, Classification, Synthesis, Properties, Characterization and applications

Detailed version

Structure of solids: Introduction to engineering materials, Description of materials science tetrahedron, Force - interatomic distance curve, Structure - description of unit cell and space lattices, Coordination number, APF for cubic and hexagonal close packed structures, Miller indices, Non crystalline structures properties of crystalline and amorphous structures, Crystal imperfections. Significance of structure property correlations in all classes of engineering materials.

Concepts of dislocations and strengthening mechanisms through alloying

Diffusion phenomenon: Rate and mechanism of diffusion, Fick's first and second law of diffusion, Applications of diffusion.

Principles of solidification and phase equilibria: Concept of free energy and entropy; Structure of liquid metals; Energetics of solidification; Nucleation and growth, Homogeneous and heterogeneous nucleation, Origination of grain and grain boundaries, Cast structure; Significance of alloying

Phase diagrams and phase transformations: Basic definitions; Gibbs phase rule, Introductions to binary systems, Construction of binary isomorphous diagram from cooling curves.

Basics of Heat Treatment: Annealing, normalising and hardening.

Ceramics: Introduction to ceramic materials; Classification of ceramics, Crystal structure and bonding of common advanced ceramic materials; Mechanical behavior of ceramics, Glass and glass ceramics, Preparation and characterisation of ceramics powders; Characterisation of ceramic materials; Applications of ceramics in advanced technologies

Books:

1. R. Abbaschian, R.E. Reed-Hill, *Physical Metallurgy Principles*, 4th ed., Cengage Learning, 2009.
2. D.R. Askeland, P.P. Phule, W.J. Wright, *The Science and Engineering of Materials*, 6th ed., Cengage Learning, 2010.

3. W.D. Callister, D.G. Rethwisch, *Materials science and Engineering: An Introduction*, 8th ed., Wiley, 2010.
4. B.S. Mitchell, *An Introduction to Materials Engineering and Science for Chemical and Materials Engineers*, 1st ed., Wiley- Interscience, 2003.
5. C. Kittel, *Introduction to Solid State Physics*, 8th ed., Wiley, 2005.
6. V. Singh, *Physical Metallurgy*, 1st ed., 2008.
7. S.H. Avener, *Introduction to Physical Metallurgy*, 2nd ed., Tata McGraw-Hill Education, 2011.
8. V. Raghavan, *Materials Science & Engineering: A first course*, 5th ed., PHI Learning, 2004.
9. W.D. Kingery, *Introduction to Ceramics*, 2nd ed., John Wiley & Sons, 1999.

CHM612

Applied Mathematics and Process Modeling

Course Description:

This course aims to introduce students to the mathematical concepts used in material processing and application of the solution techniques to various process models that have significance in material processing. This course discusses various solution techniques for ordinary and partial differential equations, numerical methods and application of these techniques for the processes involving fluid flow, heat transfer and mass transfer. The course introduces the basic laws of momentum, energy and mass transfer. Transport processes, essential for the materials processing are discussed in detail. It also covers different types of chemical reactors and their modeling and solution techniques.

Course objective:

- To introduce the students to the solution techniques for the physical models
- To develop understanding of the transport processes and chemical reactors used in material processing
- To develop modelling and computing skills

Course outcome:

- The students will develop scientific understanding of the system and core computational skill
- The students will be able to build the descriptive mathematical model of the physical system of interest and study the effect of changes in a system

Syllabus:

Mathematical concepts; Introduction to solution techniques for ordinary differential equations, Sturm-Liouville problems, Partial differential equations, Applications of PDE in heat transfer, mass transfer, diffusion, fluid flow, chemical reaction, transport process and process modeling-simulation, Boundary layer concept, balance equations for mass, momentum, energy; and estimation, Heat Transfer; Governing equations and boundary conditions; conduction, convection and radiation; Balance equations for mass transfer, Ideal reactors, Modeling of ideal reactors, solution techniques for models producing PDEs, models yielding ODEs, numerical solution methods, initial value problems, boundary value problems

Detailed version

Mathematical concepts:

Ordinary differential equations: Introduction to solution techniques for Ordinary differential equations, initial value problems, Sturm-Liouville problems, integral functions

Partial differential equations: Solution techniques for partial differential equations, separation of variables, combination of variables, Fourier integral method, Laplace transform methods

Numerical solution methods: Solution of non-linear algebraic equations, solution of linear algebraic equations, Initial value problems – Explicit integration method, Implicit integration method, Predictor corrector methods and Runge Kutta method, Boundary value problems- Linear boundary value and non-linear boundary value problems, Finite difference method for PDE

Fundamentals of transport process and process modeling: Basic laws of fluid mechanics- continuity equation, Bernoulli equation, Dimensional analysis, Principles of model development- Balance equations for mass, momentum, Energy transfer, Model development for turbulent core region, laminar sublayer region, Illustration of the Formulation Process, Combining Rate and Equilibrium Concepts, Boundary Conditions and Sign Conventions

Application of ODE/PDE: Applications of PDE in Heat Transfer, Mass Transfer, Comparison between Heat and Mass Transfer Results, Simultaneous Diffusion and Convection, Simultaneous Diffusion and Chemical Reaction, Simultaneous Diffusion, Convection, and Chemical Reaction, Heat transfer, Governing equations and boundary conditions for conduction; Transient conduction, Boundary layers, Laws of diffusion, Diffusion with and without chemical reaction, Ideal reactors: batch reactor, plug flow reactor and continuous stirred tank reactor, reactors in series; Modeling of ideal reactors and multiple reactors.

Books:

1. R. D. Rice, D. D. Do, *Applied Mathematics and Modeling for Chemical Engineers*, 2nd ed., John Wiley and Sons, 2012.
2. Norman W Loney, *Applied Mathematical methods for chemical engineers*, 2nd ed., CRC Press, 2007.
3. J.A. Dantzig, C.L. Tucker, *Modeling in Materials Processing*, 1st ed., Cambridge University Press, 2001.

References:

1. P.S. Ghosdastidar, *Computer Simulation of Flow and Heat Transfer*, Tata McGraw-Hill, New Delhi, 1998.
2. 4. J. Welty, C. E. Wicks, G. L. Rorrer, R. E. Wilson, *Fundamentals of Momentum, Heat and Mass Transfer*, 5th ed., Wiley, 2007.
3. O. Levenspiel, *Chemical Reaction Engineering*, 3rd edition, John Wiley, 1999.
4. K. Muralidhar, T. Sundararajan, *Computational Fluid Flow and Heat Transfer*, 2nd ed., Narosa Publishing House, 1995.

CHM614

Materials Characterization Techniques

Course Description:

This course comprises the fundamental principles and practical applications of different classes of materials and characterization techniques. The characterization techniques used for chemical and structural analysis of materials, including metals, ceramics, polymers, composites, and semiconductors are discussed in detail. The topics include important spectroscopic, microscopic and thermal methods for materials characterization.

Course Objectives:

- To introduce the materials characterization techniques to the students

- Help the students to understand the instrumentation aspects
- To provide a detailed understanding of data interpretation
- To provide hands on experience of the characterization techniques

Course Outcomes:

- Students will demonstrate proficiency in sample preparation methods and proper sample handling techniques.
- Students will interpret and evaluate data obtained from various analytical techniques.
- Students will identify and justify the ideal method of analysis to extract the required information.

Syllabus:

Introduction to materials and techniques; Spectroscopic methods- UV-visible and vibrational spectroscopy- Infrared and Raman, Electron spectroscopies - X-ray photoelectron spectroscopy, UV photoelectron spectroscopy, Auger electron spectroscopy; Optical microscopy, Electron microscopy- SEM, TEM; Scanning Probe Microscopies: STM, AFM; Thermal analysis- TGA, DTA, DSC; Materials analysis by Non-destructive testing (NDT).

Detailed version

Introduction: General instrumental parameters, measurement basics.

Spectroscopic methods: UV-visible spectroscopy- Beer's law, Instrumentation, Quantitative analysis; Vibrational spectroscopy- Raman and Infrared, Principles of vibrational spectroscopy, Infrared and Raman activity, Fourier transform infrared spectroscopy, Instrumentation, Raman spectroscopy, Micro Raman, Applications

Electron spectroscopies: X-ray photoelectron spectroscopy (XPS), Ultra-violet photoelectron spectroscopy (UPS), Auger electron spectroscopy (AES), Atomic model and electron configuration, Principles of XPS and AES, Chemical shift, Depth profiling, Instrumentation, Applications

Optical Microscopy: Image formation, Resolution, Aberrations, Imaging modes, Specimen preparation, Confocal microscopy

Electron microscopy: Scanning electron microscopy (SEM), Instrumentation, Electron beam-specimen interaction, Specimen preparation, Energy dispersive spectroscopy (EDS) in electron microscopes; Transmission electron microscopy (TEM) - Basics of TEM, Electron sources, Specimen preparation, Image modes, Image contrast.

Scanning Probe Microscopies: Scanning tunneling microscope (STM) and Atomic force microscope (AFM) - Working principles, working modes, Image artifacts

Thermal analysis: Thermo gravimetric analysis (TGA), Differential thermal analysis (DTA), Differential scanning calorimetry (DSC), Dynamic mechanical analysis (DMA), Thermomechanical analysis (TMA) and Dynamic mechanical thermal analysis (DMTA), Basic theory, Instrumentation and applications

Non-destructive testing: Radiography, Ultrasonic, Acoustic emission, Thermography, Holography, Basic principles, Applications in airframe and rocketry

Books:

1. Y. Leng, *Materials Characterisation: Introduction to Microscopic and Spectroscopic Methods*, John Wiley & Sons (Asia), 2008.
2. S. Zhang, Lin Li, A. Kumar, *Materials Characterisation Techniques*, CRC press, 2008.

3. D.A. Skoog, F.J. Holler, S. R. Crouch, *Instrumental Analysis*, Cengage Learning, 2007.
4. J.C. Vickerman, I. Gilmore, *Surface Analysis: The Principal Techniques*, 2nd ed., John Wiley & Sons, Inc.2009.
5. W. W. Wendlandt, *Thermal Methods of Analysis*, John Wiley, 1974.
6. B. Raj, T. Jayakumar, M. Thavasimuthu, *Practical Non-Destructive Testing*, 2nd ed., Narosa Publishing House, 2002.

References:

1. R.M. Silverstein, *Spectrometric identification of organic compounds*, 7th ed., John Wiley and Sons, 2007.
2. C.R. Brundle, C.A. Evans, S. Wilson, *Encyclopedia of Materials Characterisation*, Butterworth-Heineman, 1992.

CHM615

Nanoscience and Technology

Course Description

The course Nanoscience and technology provides an overview of nanomaterials, their synthesis, properties and specific applications of nanotechnology in electronic devices, biomedical fields, environmental solutions, and energy production. Also, it touches upon the possible applications in engineering. The course is mainly a journey through the chemistry and physics of nanoscience which explains the unique/exceptional properties of nanomaterials. Further, these properties of nanomaterials are explained with specific examples. The possible effects of nanomaterials on environment/humans are also discussed.

Objectives:

- To introduce the students to the world of nanoscience to provide understanding of the fundamentals of nanoscience
- Impart knowledge on various synthesized/developed and natural nanomaterials
- To introduce them to the unique properties of nanomaterials, Size and shape dependence of properties at nanoscale.
- To equip the students with the knowledge of methods to synthesize nanostructures and materials and make them aware, the huge potential of nanomaterials/structures in engineering/technologies

Outcome:

- Learn the significance and unique properties of nanomaterials
- Understand different types of nanomaterials and the processes for synthesizing and preparing them.
- Analyze the fundamental theories that differentiate nanomaterials from their bulk counterparts.
- Evaluate and select appropriate nanomaterials for various applications.
- Design and manipulate materials to create new nanomaterials for specialized applications

Syllabus:

Introduction- Size and shape dependent properties and the uniqueness of nanomaterials; surface characteristics and stabilization; Quantum confinement; Zero dimensional, one dimensional and two dimensional nanostructures – Synthesis/Processing of nanomaterials – top-down and bottom-up approaches– Techniques for characterization and property evaluation- applications- societal implications and risk factors

Detailed Version

General introduction and theory of nanomaterials- History of nanomaterials; Size and shape dependant properties and their uniqueness; Energy at nanoscale - surface characteristics and electrostatic and steric stabilization - Quantum confinement - zero dimensional, one dimensional and two dimensional nanostructures, metal nanoparticles, semiconductor nanocrystals (Quantum dots)

Synthesis of nanomaterials- Introduction to nanoparticle synthesis – top-down and bottom-up approaches Nucleation and growth of nanoparticles.- physical nanofabrication techniques (PVD, CVD, MBE, self-assembly & lithographic techniques) and wet chemical methods for the synthesis.

Functional nanomaterials- Synthesis, properties and applications of organic, inorganic, hybrid nanomaterials, self-assembled nanostructures, Carbon based nano materials: fullerene, carbon nanotube, graphene, carbon onion, nanodiamond and films; Biomimetic nanomaterials - introduction to biomimetics, mimicking mechanisms in nature, synthesis and applications of bioinspired nanomaterials.

Applications of nanomaterials- Application of nanomaterials in healthcare, coatings, environment, catalysis, agriculture, automotive, sensors, electronics, photonics, energy and aerospace sectors.

Books:

1. Y. Yin, Y. Xia, *Encyclopedia of Nanomaterials*, Elsevier, 2023.
2. Bharat Bhushan, (Ed.), *Handbook of Nanotechnology*, Springer, 2016.
3. Carl C. Koch (Ed.), *Nanostructured Materials: Processing Properties and Applications*, William Andrew Inc., 2007.
4. Anke Krueger, *Carbon Materials and Nanotechnology*, Wiley-VCH Verlag GmbH & Co. KGaA, 2010.
5. Cao, G., *Nanostructures and Nanomaterials Synthesis, Properties, and Applications*, Imperial College Press, 2004.
6. Garcia-Martinez, J., (Ed.), *Nanotechnology for the Energy Challenge*. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2009.
7. Goddard III W.A., et. al.,(Ed.), *Handbook of Nanoscience, Engineering, and Technology*, Taylor & Francis Group, 2007.
8. B.P.S. Chauhan (Ed), *Hybrid Nanomaterials: Synthesis, Characterization, and Applications*,Wiley-VCH Verlag GmbH, 2011.
9. J. Lei and F.Lin, *Bioinspired Intelligent Nanostructured Interfacial Materials*, World Scientific Publishing Company, 2010.
10. Challa S. S. R. Kumar (Ed.) *Biomimetic and Bioinspired Nanomaterials*, Wiley-VCH Verlag GmbH, 2010.

CHM621

Processing and Design of Materials

Course Description:

This course focuses on the various processing techniques for metals, polymers and ceramics. The process parameters involved in the processing and their influence on the final shape of the product is discussed. Design of tools and other accessories for manufacturing a healthy product is also included.

Course Objectives:

- To impart basic knowledge on the manufacturing techniques of various materials.

Course Outcomes:

- Students will compare and contrast various manufacturing techniques to obtain simple and complex shapes, and apply appropriate techniques to produce desired shapes

Syllabus

Introduction to materials processing; **Polymer processing** - rheology of polymeric materials, Compounding and processing of plastics and rubbers, fiber spinning and manufacturing processes. **Ceramic processing**- Pressing, CIP, HIP, Slurry processing, Slip casting, Pressure casting, Tape casting, Gel casting, Rapid prototyping, Sol-gel processing, Thermal and plasma spraying, Thick and thin film coatings; **Processing of Metallic materials**-, Casting processes, Casting design and defects; Fundamentals of deformation processing, Hot and cold working, Metal joining process, Design aspects, Materials selection and design, Weighting factors, Materials performance index; Design of engineering structures, Case studies, Modern metallic, Ceramic, Polymeric and biomaterials devices and components

Detailed version

Introduction: Materials processing science with special emphasis on processing of polymers, ceramics and metals

Polymer processing: Rheology of polymeric materials, Compounding of plastics, processing techniques: Compression, Transfer, injection, blow molding, Extrusion, Calendaring, Thermoforming, Rotational molding, Compounding and processing of rubber (both latex and dry rubber) with different formulations: Casting, rubber extrusion, Dip coating (gloves, balloons etc.), fibre spinning and manufacturing processes.

Ceramic processing: Processing of traditional ceramics- spray granulation, Pressing, CIP, HIP, Slurry processing, Slip casting, Pressure casting, Tape casting, Gel casting, Injection molding, Extrusion; Rapid prototyping through Additive manufacturing, Electrophoretic deposition, Production of ceramic fibres, Electro-spinning; Drying, Binder burnout, Green machining, Sintering; Sol-gel processing, Thermal and plasma spraying, Thick and thin film coatings- PVD and CVD techniques; Vapor infiltration techniques

Metallic processing: Casting process- major casting techniques, Solidification and volume shrinkage, Casting design and defects, Fundamentals of deformation processing, Deformation work, Hot and cold working, Few forming processes and defects;

Metallic processing: Casting process- major casting techniques, Solidification and volume shrinkage, Casting design and defects, Fundamentals of deformation processing, Deformation work, Hot and cold working, Few forming processes and defects; Metal joining process- Weldability, Concepts of Fusion and solid state welding processes.

Design aspects: General principles of materials selection and design based on requirements of function, Property, Processability and cost; Quantitative methods of materials selection, Materials performance index; Design of engineering structures from the atomic- and nano-scales to macroscopic levels; Case studies- modern metallic, ceramic, polymeric and biomaterials devices and components

Books:

1. P. Boch, J-C. Nièpce, *Ceramic Materials: Processes, Properties, and Applications*, Wiley-ISTE, 2007.
2. J-H. He, *Electrospun Nanofibres and Their Applications*, Smithers Rapra Technology, 2008.
3. Z. Tadmor, C.G. Gogos, *Principles of Polymer Processing*, 2nd ed., Wiley International, 2006.
4. T.A.Osswald, *Polymer Processing Fundamentals*, Hanser Publications, 1998.
5. M.N. Rahaman, *Ceramic Processing and Sintering*, 2nd ed., CRC press

6. F.C. Campbell, *Elements of Metallurgy and Engineering Alloys*, ASM International, 2008.
7. J. Beddoes, M.J. Bibby, *Principles of Metal Manufacturing Processes*, Elsevier, 2003.
8. G.E. Dieter, *Mechanical Metallurgy*, McGraw-Hill, 3rd ed., 1986.
9. E. Degarmo, J.T. Black and R.A. Kohser, *Materials and Processes in Manufacturing*, 9th ed., Wiley, 2002.
10. S. Kalpakjian, S.R. Schmid, *Manufacturing Engineering and Technology*, 6th ed., Pearson, 2009.

CHM623

Composite Science and Technology

Course Description:

Composites are one of the most important classes of materials. The course 'Composite Science and Technology' is intended to give thorough understanding about this class of materials, especially polymer matrix composites and carbon-carbon composites. Students will be introduced to the advantages of the use of different types of composites, their manufacturing, properties and applications. Testing and applications of these composites including aerospace applications are discussed.

Course objectives:

- To provide knowledge on the advantages of use of different types of composites
- To make the students familiar with the mechanism of reinforcement and failure of composites
- To make them aware the manufacturing and testing methods of composites

Course outcome:

- Students will explain and appreciate the significance of composites as an important class of materials.
- Students will design and develop composites for specialized applications.
- Students will select and justify appropriate characterization methods for different classes of composites

Syllabus

Introduction to Composite Materials, Classification, reinforcement; Polymer matrix composites, Thermoplastic and thermosetting resins, Common matrix reinforcement system; Concept of A stage, B stage and C stage resins; Particulate and fibre filled composites, Short fibre composites, Theories of stress transfer; Continuous fibre composites, Failure mechanism and strength, Halpin-Tsai equations, Prediction of Poisson's ratio, Various failure modes; Specialty composites, Composites for satellites and advanced launch vehicles, Design considerations, PMC- for structural composites, Nanocomposites, Design and analysis of composite structures macro mechanics, Micro mechanics, Laminate analysis, FE model and analysis, Manufacturing techniques, Testing of composites, Raw material testing

Detailed version

Introduction to composite materials: Definition of composites, Classification of composites; General characteristics of reinforcement- classification, terminology used in fiber science, CMC, MMC and PMC.

Polymer matrix composites: Thermoplastic and thermosetting resins; Commonly used matrix reinforcement system; Fibre, Flake and particulate reinforced composites, Reinforcements used in PMC's-

glass, carbon, aramids, boron, Roving's, yarns, fabrics, etc.; Thermoset matrices for aerospace components- polyesters, epoxies, phenolics, vinyl esters, cyanate esters, etc.; Thermoplastic matrices for advanced composites- PEEK, polysulfones, polyimides, etc. concept of A stage, B stage and C stage resins

Particulate and fiber filled composites: Applications, Function of matrix, Function of fibers, Polymer-fiber interface, Factors influencing the performance of composite, Coupling agents, Bonding agents, Short fiber composites, Theories of stress transfer, Analysis of short fiber composites, Critical fiber length, Rule of mixtures

Continuous fiber composites: Analysis of long fiber composites, Longitudinal behavior of unidirectional composites; Failure mechanism and strength, Factors influencing longitudinal and transverse strength and stiffness, Halpin-Tsai equations for transverse modulus, Prediction of Poisson's ratio, Various failure modes

Specialty composites: Composites for satellites and advanced launch vehicles, Design considerations PMC- for structural composites, Theory and application of ablatives.

Nanocomposites: Nano particle dispersion in polymer matrix, Polymer- nanoclay composites and polymer-carbon nanotubes composites

Design and analysis of composite structures: Macro mechanics of a lamina, Micro mechanics, Laminate analysis, FE model and analysis

Manufacturing techniques: Hand lay-up, Filament winding, Pultrusion, Resin transfer molding, Processing science of reactive polymer composites, Process steps for production, Selection of processing conditions toolings, Equipments, Carbon-carbon composites, Processing, Thermal and mechanical properties, Quality control

Testing of composites: Raw material testing, Property evaluation at laminate level, NDT techniques

Books:

1. R.M. Jones, *Mechanics of Composites*, 2nd ed., Taylor & Francis, 1999.
2. T. G. Gutowski, (Ed.) *Advanced Composites Manufacturing*, John Wiley & Sons, New York 1997.
3. P.M. Ajayan, L. Schadler, P.V. Braun *Nano Composite Science and Technology*, Wiley VCH, 2003.
4. E. Fitzer, L.M. Manocha, *Carbon Reinforcement and Carbon/Carbon Composites*, Springer-Verlag, Heidelberg, New York, 1998.
5. K.K. Chawla, *Ceramic Matrix Composites*, Kluwer Academic Publishers, 2003.
6. N. Chawla, K.K. Chawla, *Metal Matrix Composites*, Springer-Verlag, 2006.
7. J.C. Seferis, L. Nicolais, (Eds.) *The Role of the Polymeric Matrix in the Processing and Structural Properties of Composite Materials*, Plenum Press, New York 1983.

CHM624

Aerospace Materials

Course Description:

Aerospace materials are light-weight structural materials capable of withstanding severe environments and extreme stress levels. The course is intended to provide an overview of metallic, ceramic, polymeric and composite materials used for construction of spacecraft and their composition-structure-processing-property correlation.

Course objectives:

- To introduce the students to various classes of materials used in aerospace
- To understand the materials used and their property requirements for different parts of spacecraft

- To study composition- structure-processing-property correlation in aerospace materials to enable them to design new materials with improved property.

Course outcome:

- Students will identify and categorize different classes of aerospace materials."
- Students will analyze and explain the property requirements of materials used in different areas of a spacecraft."
- Students will evaluate the composition-structure-processing-property correlation of aerospace materials to design new materials with improved properties

Syllabus:

Carbon based materials- carbon fiber, carbon-carbon composites, carbon aerogels and foams, Ceramic materials- polymer derived ceramics, ceramic fibers, ceramic matrix composites, thermal barrier coatings, ceramics aerogels and foams, Ultrahigh temperature ceramics; materials with zero thermal expansion, Metallic materials- Evolution of materials for aerospace sectors, super alloys, titanium alloys, intermetallics and metal matrix composites; High temperature polymers- aromatic liquid crystalline polyesters, polyamide, phenolics, polyimide, poly ether ether ketones; Materials for cryogenic application, Materials for space environment, Materials for spacecraft, Functionally graded materials. Space worthiness of materials.

Detailed version

Carbon based materials: Carbon fiber- precursors and production, properties; carbon-carbon composites- production, properties and applications; Carbon aero-gels; Carbon foams;

Ceramic materials: Polymer derived ceramics- synthesis, processing of pre-ceramic polymers, ceramic fibers, Ceramic matrix composites, Thermal barrier coatings, Ablative materials, Silica tiles, Ceramic aerogels, Porous ceramics and ceramic foams, Ultrahigh temperature ceramics- TiB_2 , ZrB_2 , HfB_2 and their composites, Materials with zero thermal expansion-glass ceramics-preparation and application

Metallic materials:

Historical evolution of aerospace materials, Certification and testing of Aerospace materials.

Metallic materials: Aluminum alloys, Super alloys, - microstructure, properties and applications

High temperature polymers: Aromatic liquid crystalline polyesters, Phenolics, Polyimide, Poly ether ether ketones- synthesis, processing and applications

Materials for cryogenic applications: Metals for low temperature applications, Austenitic stainless steel, Nitrogen containing steel, Aluminium, Aluminium-lithium alloys, Titanium alloys, Cryo insulation materials, Polymers and adhesive for cryo temperature applications

Materials for space environment: Radiation shielding materials, Atomic oxygen resistant materials, Space suit materials and materials for life support systems, Evaluation of materials for space environment and space worthiness.

Books:

1. G. Savage, *Carbon-Carbon Composites*, 1st ed., Chapman and Hall, 1993.
2. M. Scheffler, P. Colombo, *Cellular Ceramics, Structure, Manufacturing, properties and Applications*, 1st ed., Wiley-VCH, 2006.
3. W.D. Kingery, H.K. Bowen, D.R. Uhlmann, *Introduction to Ceramics*, 2nd ed., Wiley-Interscience, 1976.
4. J.S. Reed, *Principles of Ceramic Processing*, 2nd ed., Wiley-Interscience, 1995.

5. H.M. Flower, *High Performance Materials in Aerospace*, 1st ed., Chapman & Hall, 1995.
6. B.Horst, B. Ilschner, K.C. Russel, *Advanced Aerospace Materials*, Springer-Verlag, Berlin, 1992.
7. F. Mohammad, *Speciality Polymers: Materials and Applications*, I.K. International publishing House Pvt. Ltd , 2007.
8. W. Krenkel, R. Naslain, H. Schneider, (Eds.) *High Temperature Ceramic Matrix composites*, 1st ed., Wiley-VCH, 2006.
9. T.W. Clyne, P.J. Withers, E.A. Davis, I.M. Ward, *Introduction to Metal Matrix Composites*, *Cambridge Solid State Science Series*, 1st ed., Cambridge University Press, 1993.
10. R.R. Luise, *Applications of High Temperature Polymers*, CRC press, 1st ed., 1996.

Elective courses (total 16 courses)

CHM861

Biomaterials

Course Description:

Biomaterials are materials which are engineered to interact with biological systems for a medical purpose - either a therapeutic or a diagnostic one. Biomaterials science is a growing field of materials science and deals with study and development of different classes of materials to replace or augment human tissues. The course is intended to give an overview of the fast growing field of biomaterials. Different classes of biomaterials, testing, toxicology and characterizations, materials for drug delivery, nanobiomaterials and smart biomaterials are included in the course contents. Tissue engineering which is the ultimate solution for organ replacement is also introduced.

Course objectives:

- To introduce students to various classes of biomaterials
- To develop understanding regarding the characteristics of the materials to be used as biomaterials
- To make them aware the growing applications and possibilities of biomaterials to enhance the quality of life.

Course outcome:

- Students will get introduced to different classes of biomaterials and their applications
- The vast applications of biomaterials will encourage students to explore them in detail and to design and engineer synthetic and natural materials for biomedical applications
- The course would also enable the students to appreciate the role of tissue engineering as a tool to enhance the quality of life.

Syllabus:

Introduction to classes of materials used in medical applications-Testing of biomaterials- Toxicology- Polymeric drug delivery systems - Metals and ceramics - Dental materials-Smart biomaterials- Nanobiomaterials - Nanogels and microgels- Tissue engineering.

Detailed syllabus

Biomaterials: Introduction to classes of materials used in medical applications: Metals, polymers, ceramics, bioresorbable and biodegradable materials, coatings, medical fibers, non fouling surfaces.

Testing of biomaterials: In Vitro and in vivo assessment of tissue compatibility. Testing of blood-materials interactions. ISO standards for testing of blood compatibility and tissue compatibility. Degradation of

materials in the biological environment: Effects of the Biological environment on metals, polymers and ceramics. Relevant international standards: ISO, FDA and ASTM

Toxicology: cytotoxicity, systemic effects, genotoxicity, carcinogenicity, reproductive toxicity, sensitization & irritation, tissue compatibility and inflammatory response, evaluation of host response.

Metals and ceramics: stainless steels, cobalt based alloys, titanium based alloys, characteristics and processing of bioceramics, nearly inert crystalline ceramics, porous ceramics, bioactive glasses and glass ceramics, calcium phosphate ceramics, calcium phosphate coatings, resorbable calcium phosphates, clinical applications of hydroxyapatite. Pyrolytic carbon.

Dental materials: Introduction to dental materials polymers, ceramics and metals, applications of dental materials, physico-chemical, mechanical, toxicological and in vitro clinical performance of dental materials and implants.

Polymers in drug delivery : Introduction to polymeric drug delivery systems, Targeted drug delivery. Passive or active targeting, targeting tumor cells, polymer-protein conjugates, polymer drug-conjugates. Pharmacokinetics. Application of hydrogels in controlled drug delivery systems.

Smart biomaterials: Stimuli responsive polymers (pH, temperature, light, magnetic and biomolecules) and their applications as biomaterials. Stimuli responsive hydrogels.

Nanobiomaterials: Interaction of bio-molecules and nano particle surfaces. Biocompatible nanomaterials, Nanogels and microgels: preparation methods, characterization and applications.

Tissue engineering : Introduction to the basic concepts of scaffolds in tissue engineering. Functions and requirements of scaffolds in tissue engineering.

Natural and synthetic materials for tissue engineering scaffolds. Application of hydrogels in tissue engineering. Processing techniques for scaffold preparation such as solvent casting and particulate leaching, freeze drying, phase separation, gas foaming, solid freeform fabrication, self-assembled materials-3D bioprinting.

Text Books:

1. B. Ratner, A. Hoffman, F. Schoen, J Lemons, *Biomaterials Science: An introduction to materials in Medicine*. 2nd edition, Academic Press, 2004.
2. S. Dumitriu, 2nd edition, *Polymeric Biomaterials*. Marcel Dekker, 2002
3. C. T. Laurencin, L. S. Nair, *Nanotechnology and Tissue Engineering, The Scaffold*, CRC Press, 2008
4. S. Ramakrishna, T. S. Sampath Kumar, *Biomaterials: A nano approach*. CRC press, 2010
5. I. Galaev, Bo Mattiasson, *Smart Polymers: Applications in Biotechnology and Biomedicine*, 2nd Edition, CRC Press, 2007
6. S. Li, A. Tiwari, M. Prabakaran and S. Aryal, *Smart Polymer Materials for Biomedical Applications (Materials Science and Technologies)*, Nova Science Publishers Inc, 2010
7. M. De Villiers, P Aramwit and G S. Kwon, *Nanotechnology in drug delivery*. Springer, 2009.
8. A. Kirkland and J. Hutchison, *Nano characterization*, RSC publishers, 2007.

Course Description:

Soft materials are ubiquitous in nature and living organisms achieve their functionality by controlling the structure and properties of these materials over a hierarchy of length scales, from single molecules to tissues. Recently, the importance of soft materials in the industrial sector, especially medical, pharmaceutical and food industries has increased tremendously. Hence the course aims to discuss on this interdisciplinary domain bridging chemistry, physics, biology and materials science and engineering by using polymers,

colloids, foams, gels, biological tissue as typical examples. From the molecular components to the highly complex hierarchical architecture, the significance of designing the fundamental building blocks and the forces behind self-assembly will be discussed. The instrumental techniques for characterization of soft materials will also be dealt with. There will be lab sessions (announced) for selected topics.

Course Objectives:

- To underpin the significance of soft materials in controlling complex living systems
- To make students aware of the various classes of soft materials
- To signify the role of self-assembly and the formation of varied architecture
- To introduce the various instrumental characterization techniques for soft materials (couple of lab sessions will be organized)

Course Outcome:

- Students will develop a fundamental understanding of the various classes of soft materials that are relevant for technological applications in different sectors including materials industry and consumer products.
- Students will appreciate the role of molecular units in the design of soft materials and understand the process of self-assembly.
- Students will get exposed to synthesis, processing and characterization of soft materials during the laboratory sessions planned along with the course.
- The minor projects/technical report writing will ensure the development of proficiency in scientific English and help to advance students' soft skills

Syllabus:

Fundamentals of chemistry of soft materials; Basic concepts of soft materials, Various interactions, Photoresponsive molecules and self-assembly, Micelles, Vesicles, Toroids, Colloids, Rods, Examples of molecules forming soft materials, Instrumental techniques for morphology studies of soft materials, Liquid crystals, Different class of gels- low molecular weight organo gels, hydrogels, basics, classifications, behaviour of soft materials under zero gravity.

Detailed version

Fundamentals of supramolecular chemistry of soft materials: The concept and development of soft materials, Nature of supramolecular interactions for the soft materials; Noncovalent interactions, ion-ion interactions, Ion-dipole interactions, Dipole-dipole interactions, π - π stacking, Cation- π interactions, Solvophobic interactions; van der Waals interactions, Hydrogen bonding, Multiple hydrogen bonding motifs, Jorgensen model for H-bonding; Photoresponsive molecules and self-assembly, Micelles, Vesicles, Toroids, Colloids, Rods

Self-assembly of supramolecular soft architectures: The concept of supramolecular self-assembly- one, two and three dimensional self-assemblies, Phthalic acid based self-assemblies, Cyanuric acid-melamine assemblies, Rosette motifs, Hierarchical self-organization, Perylenebisamide-melamine assemblies, Oligo(p-phenylenevinylene and p-phenyleneethynylene) self-assemblies, Supramolecular polymers resulting from quadruple H-bonding modules, Molecular capsules, Self-assembled dendrimers, Self-assembled nanotubes; Molecular motors; Liquid crystals.

Gels: Different class of gels- low molecular weight organo gels, hydrogels, basics, classifications, Structure and theory of formation, Swelling, Physical hydrogels, Ionic and hydrogen bonding in gels, Polyelectrolyte gels, Coacervates, Covalently bonded hydrogels, Applications of hydrogels
Behaviour of soft materials under zero gravity.

Books:

1. J. -M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, Wiley VCH Verlag, 1995.
2. J. Steed, J. L. Atwood, *Supramolecular Chemistry*, 2nd ed., John Wiley, 2009.
3. J. Steed, J.L. Atwood, *Organic Nanostructures*, 2nd ed., Wiley VCH Publishers, 2008.
4. V. V. Tsukruk, S. Singamaneni, *Scanning Probe Microscopy of Soft Matter: Fundamentals and Practices*, Wiley VCH Publishers, 2011.
5. N. Takashi, *Supramolecular Soft Matter*, 1st ed., John Wiley & Sons, 2011.
6. V.K. Pillai, M. Parthasarathy, *Functional Materials: A Chemist's Perspective*, Orient BlackSwan, Universities Press- IIM Series, 2013.
7. S. K. Tripathy, Jayant Kumar, H.S. Nalwa, *Handbook of Polyelectrolytes and Their Applications*, American Scientific Publishers, 2003.
8. B. Rolando, *Hydrogels Biological Properties and Applications*, 2nd ed., Springer, 2009.
9. M. Tokita, K. Nishinari, *Gels: Structures, Properties, and Functions: Fundamentals and Applications in Vol. 136 of Progress in Colloid and Polymer Science*, Springer, 2009.

CHM863**Computational Materials Science****Course Description:**

The basic microscopic constituents of materials being atoms and inter atomic interactions being responsible for the macroscopic behaviour and properties of a material, performing computer simulations in materials across several characteristic length and time scales has obvious appeal as a valid tool aiding technological innovation. This basic course is framed so as to benefit science students who aim at material discoveries and technologists who seek optimised materials for their application of choice. The course will bring out the various facets of computational materials science such as acting as the link between analytic theory and experiment, a tool to scrutinize theories, and as an exploratory research tool for predicting experiments in a laboratory which are difficult to realise physically. The topics are chosen and hierarchically arranged so as to lay strong foundations of computational science in students of graduate and post graduate level.

Course Objectives:

- To introduce students to the fundamental aspects of computational science and its increasing role in the development and optimization of materials.
- Provide a combination of theory and laboratory activities for establishing the potential of computational tools in novel materials' design.
- To help students become aware of the various tools available for materials discovery and optimization.

Course Outcomes:

- Students will get introduced to the new interdisciplinary field of computational materials science and engineering.
- Students gain an understanding of the theory behind computations and various tools relevant to the design of future materials.

Syllabus:

Introduction to computational modeling and simulation for Materials Science. Molecular mechanics, Density functional theory (DFT), Molecular dynamics (MD), Monte Carlo (MC) methods, introduction to

quantum MC methods, analysis exercises using softwares, Materials genomics, High through-put combinatorial algorithms for materials design.

Detailed version

Introduction to computational modeling and simulation for Materials Science, First principle methods: the beginnings of Quantum mechanics, Schrodinger wave equation, time-independent wave equation, Molecular mechanics- Force Field Methods, Postulates of quantum mechanics, Energy Hamiltonian, early first principles calculation, Born-Oppenheimer approximation, Hartree method (one electron), Hartree-Fock molecular orbital theory, Self-consistent-field (SCF) procedure;

Density functional theory (DFT): electron density in DFT, Hohenberg-Kohn theorems, Kohn-Sham approach, exchange correlation functionals, solving Kohn-Sham equations, DFT extensions and limitations. DFT exercises using software (VASP/Gaussian).

Molecular dynamics (MD): Atomic model in MD, Molecular mechanics, potentials, solutions for Newton's equation of motion, running MD: initialization, pre-set ups, periodic boundary condition, positions and velocity, time steps, ensembles, integration equilibration, minimisation in static MD run – steepest descent method, conjugate gradients method, run analysis. MD analysis exercises using software (LAMMPS/ XMD)

Monte Carlo (MC) methods: Basis of MC methods, stochastic processes, Markov's process, ergodicity; Algorithms for MC simulations, random numbers, sampling techniques. Applications of MC methods: System of classical particles, percolation, polymer systems, nucleation, crystal growth, fractal systems. Limitations of MC methods, introduction to quantum MC methods.

Materials genomics: High through-put combinatorial algorithms for materials design.

Text Books:

1. Richard LeSar, Introduction to Computational Materials Science: Fundamentals to Applications, Cambridge University Press, 2013.
2. June Gunn Lee, Computational Materials Science: An Introduction, CRC Press, (I edn) 2012; (II edn 2016)

References:

1. Kaoru Ohno, KeivanEsfarjani, Yoshiyuki Kawazoe, Computational Materials Science: From Ab Initio to Monte Carlo Methods, 2nd Ed., Springer, 2018.
2. I.N. Levine, Quantum Chemistry, 6th ed., Prentice Hall, 2009.
3. J.A. Dantzig, C.L. Tucker, Modeling in Materials Processing, 1sted., Cambridge University Press, 2001
4. Guillermo Bozzolo, Ronald D. Noebe, Phillip B. Abel (Editors), Applied Computational Materials Modeling: Theory, Simulation and Experiment, Springer, 2007.
5. A.R. Leach, Molecular modeling: Principles and Applications, 2nd ed., Pearson-Prentice Hall, 2001.

Course Description:

The propellants and explosives are extensively used for various military & space applications. This course intends to cover the classification of the various propellants & propulsion systems with their key applications, definitions, thermochemistry of chemical propellants, manufacturing, properties and

processing of propellants and explosives and their end use. The additives and eco-friendly propellants which play a vital role in augmenting the performance of futuristic propellants for various missions are discussed.

Course Objectives:

- To introduce the basic principles of propulsion and chemical propellants to the students
- To make them understand the importance of propellant composition & processing to achieve required propulsion parameters.
- To develop professional competence in the area of rocket propellants and space ordinance systems.

Course Outcomes:

- Students will get the knowledge and understanding of the key mechanisms and materials used in rocket propulsion.
- Students will appreciate the significance and application of rocket propulsion to launch vehicles.

Syllabus

Classification of chemical propellants; Liquid propellants- mono propellants and bi propellants, Oxidizers and fuels; Liquid engines and solid motors, Selection criteria for oxidizers and fuels, Solid Propellants- Ingredients of composite propellants, Oxidizers and cross-linked binders, Green propellants, Advanced and futuristic Propellants; Propellant processing, Ballistic properties, Characterization of solid propellant, Solid motor subsystems; Space ordinance systems- introduction to explosives

Detailed version

Fundamentals of rocket propulsion: Working of propellants- characteristics velocity and specific impulse, Selection criteria for oxidizers and fuels, Bond energy and thermo chemistry, Classification of chemical propellants

Liquid propellants: Liquid engines- liquid propellants feed systems, liquid engine cycles, mono propellants, bi propellants- earth storable-cryo and semi cryo systems, Oxidizers- LOX and oxides of nitrogen, Fuels: LH₂, Hydrocarbons - Isosene and hydrazines, Cryogenic Propellants, Ecofriendly propellants, futuristic propellants, Advanced oxidizers and fuels, Gelled propellants.

Solid propellants: Homogeneous and composite solid propellants, Ingredients of composite propellants- oxidizers, selection criteria- nitrates, perchlorates and advanced oxidizers, ADN and HNF- manufacturing of ammonium perchlorate, High energy additives, Cross-linked binders- polyurethanes, carboxyl and hydroxyl terminated polybutadiene prepolymers, Manufacturing of HTPB, Functionality distribution of HTPB, High energy binders; azido and oxitane polymers, Curatives, Plasticizers and bonding agents, Propellant processing- pot life and cure time, Solid motors and grain configuration, Burning rate and burning rate law, Ballistic modifiers, Characterisation of solid propellant, Mechanical properties and structural integrity; Solid motor subsystems- Insulation, Inhibition and liner systems, Motor case and nozzle hardware

Space ordinance systems: Introduction to explosives- deflagration and detonation, Classification of explosives, Common explosive compounds- nitrate esters, nitro compounds and nitramines, Igniters, Safety of propellants and explosives

Books:

1. G. P. Sutton, O. Biblarz, *Rocket Propulsion Elements*, 7th ed., John Wiley & Sons, 2001.
2. S. F. Sarnar, *Propellant Chemistry*, Reinhold Publishing Co., 1966.
3. C. Boyars, K. Klager, *Propellants Manufacture, Hazards and Testing*, in Advances in Chemistry Series 88, American Chemical Society: Washington DC, 1969.

4. H. Singh, H. Shekhar, *Science and Technology of Solid Rocket Propellants*, Printwell, Darbhanga, 2005.
5. K. Ramamurthi, *Rocket Propulsion*, Macmillan Publishers, 2010.
6. Kirk- Othmer *Encyclopedia of Chemical Technology*, Vol. 10, *Explosives and Propellants*

References (for selected topics):

1. Y. Vigor, T.B. Brill, R. We-Zhen, *Solid Propellant Chemistry, Combustion and Motor Interior Ballistic*, Progress in Astronautics and Aeronautic, Vol. 185, AIAA, 2000.
2. L. Nielsen, R.F. Landel, *Mechanical Properties of Polymers and Composites*, 2nd ed., Marcel Dekker Inc., New York, 1994.
3. T. Urbanski, *Chemistry and Technology of Explosives*, Vol. I to IV, Pergamon Press.

CHM865

Thin Films and Surface Engineering

Course description:

Thin film and surface engineering is a sub-discipline of Materials Science and Technology which plays an important role in the development of new material with unique properties required for specific applications. This course provides an introduction to various surface modification methods and thin film deposition techniques. This course discusses difference between various vacuum based deposition techniques, surface characterization, evaluation of surface modified materials, effect of deposition techniques/surface modification methods on properties and structure of film and surface engineered properties. Latest developments in thin film technology and surface engineering of materials and their application will also be discussed in this course.

Course objective:

- To develop understanding of various surface modification techniques to improve the surface properties and to evaluate their properties
- To provide a comprehensive overview of the latest developments in thin films
- To develop competence and skills to select the suitable thin film deposition techniques/surface modification methods for a certain application

Course outcome:

- The students will have knowledge and understanding of necessity of thin films
- The students will be aware of the role of surface engineering of materials to modify/improve the surface properties
- The students will be able to select the suitable thin film deposition technique/surface modification method to achieve the required surface property

Syllabus:

Surface modification techniques, Surface modification of ferrous and nonferrous metals, Surface engineering by energy beams, Film deposition techniques- Physical method of film deposition, chemical method of film deposition, Other deposition techniques, Inter-diffusion, reactions and transformations in thin films, Properties and characterization of thin films, Surface engineering of nanomaterials microencapsulation, nanostructured coatings.

Detailed version

Surface modification techniques: Surface engineering by material removal and material addition; Surface modification of ferrous and nonferrous metals- carburizing, nitriding, cyaniding, hot dipping, galvanizing, chromating, anodizing, phosphating of aluminium; Surface engineering by energy beams, Plasma for surface engineering, Laser assisted surface modification

Film deposition techniques: Sputter deposition of thin films and coatings by RF, MF, DC, Magnetron, Pulsed laser, Ion beam, Ion implantation, electroplating, electroless plating, electro polishing, electroforming, chemical vapour deposition (CVD) and plasma enhanced CVD, atomic layer deposition, atomic layer chemical vapour deposition, molecular beam epitaxy, lithography, Langmuir Blodgett, Spin coating

Inter diffusion, reactions and transformations in thin films: Fundamentals of diffusion, Inter-diffusion in thin metal films, Mass transport in thin films; Properties and characterisation of thin films- optical, electrical, mechanical and magnetic, structural morphology of deposited films and coatings

Surface engineering of nanomaterials: Hybridization of nanomaterials, microencapsulation, synthesis, processing and characterization nano structured coatings and their application

Text Books:

1. Modern Surface Technology, Edited by Friedrich-Wilhelm Bach, Andreas Laarmann, and Thomas Wenz, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 2006
2. M. H. Francombe, S. M. Rossnagel, A. Ulman, Frontiers of Thin Film Technology, Vol. 28, Academic press, 2001.

Reference:

3. K. L. Chopra, Thin Film Phenomena, McGraw Hill, 1979. R.F. Bunshah, Deposition Technologies for Films and Coatings, Noyes Publications, New Jersey, 1982.
4. M. Ohring, Materials Science of Thin Films, 2nd ed., Academic Press, San Diego, 2002.
5. F. A. Lowenheim, Electroplating, McGraw Hill, New York, 1978.
6. B. Bhushan, Introduction to Tribology, John & Sons, New York, 2002.
7. G.W. Stachowiak, A.W. Batchelor, Engineering Tribology, 3rd ed., Elsevier-Butterworth-Heinemann, 2005.
8. ASM Metals Handbook, Surface Engineering, American Society for Metals, Vol.5, 9th ed., 1994.
9. Nanomaterials and Surface Engineering, Edited by Jamal Takadoum, John Wiley & Sons, Inc., USA

CHM866

Mechanical Behaviour of Materials

Course Description:

The course focuses on the response of materials to external loads. The theory of elasticity, plasticity and concepts of fracture mechanics will be dealt together. The behavior of materials under dynamic loading and at higher temperatures will also be discussed. The strengthening mechanisms of various materials will be discussed.

Course Objectives:

- To impart basic knowledge on the response of the materials under static/dynamic loading at different temperatures.

Course Outcomes:

- The students will have insights on the basic deformation behavior of various materials

- They will be able to make the right choice of material for a given loading conditions.

Syllabus:

Review of structure and bonding in materials; Elastic, plastic and visco-elastic behavior; Yield criteria, failure, ductile to brittle transition; Linear elastic fracture mechanics; Elastic-plastic fracture mechanics-strengthening mechanisms, fatigue, creep; Super plasticity- tests of plastic behavior, embrittlement of materials

Detailed version

Introduction to mechanical response of materials: Bonding and young's modulus, anelasticity, Theoretical estimates of yield strength in metals and ceramics.

Mechanical behaviour of polymers: structure of polymers, elastic and plastic response, deformation mechanisms, time dependent deformation, visco elastic models.

Dislocation theory and strain hardening in metals and ceramics: Burgers vector, stress field, forces on dislocations, dislocation jogs and kinks, frank reed source, Lomer-cottrell lock, strain hardening behaviour, twinning, yield point elongation, strain ageing, serrated flow.

Fatigue: characteristics of fatigue fracture, Influence of residual stresses, fatigue terminology, strain life equation, cumulative damage, stages of crack growth, crack growth rate, factors affecting fatigue life.

Creep: High temperature materials, creep curve, structural changes during creep, creep mechanisms, deformation mechanism map, creep fracture, creep in polymers and ceramics, Larsen miller parameter.

Fracture: Griffith's theory, fracture toughness, strain energy release rate, crack growth in ductile and brittle materials, types of fracture (mechanisms of ductile and brittle fracture), notch effect, fracture in ceramics and composites.

Books:

1. G.E. Dieter, *Mechanical Metallurgy*, 2nd ed., McGraw-Hill, 1976.
2. R.W. Hertzberg, *Deformation and Fracture Mechanics of Engineering Materials*, John Wiley & Sons, 1989.
3. J. Roesler, H. Harders, M. Baeker, *Mechanical Behaviour of Engineering Materials: Metals, Ceramics, Polymers, and Composites*, Springer-Verlag, 2007.

Reference:

1. T. H. Courtney, *Mechanical Behavior of Materials*, McGraw-Hill, 1990.
2. R. Hill, E. Robert, *Physical Metallurgy Principles*, 2nd ed., East West Press, 1972.
3. W.M. Hyden, W.G. Moffatt, *Structure and Properties of Materials*, Vol. 3, McGraw Hill
4. M.A. Meyers, K.K. Chawla, *Mechanical Behavior of Materials*, 2nd ed., Cambridge University Press, 2009.
5. W.F. Hosford, *Mechanical Behavior of Materials*, Cambridge University Press, 2005.
6. R.W.K. Honeycombe, *Plastic deformation of Metals*, 2nd ed., Edward Arnold Press, 1984.

CHM867

Paints and Coatings

Course Description:

Paints and coatings provide the primary functions of decoration and protection and are of considerable economic and social importance. The major development that has taken place in the field of coatings during the last decade has been the adoption of the new coating technologies. The current course intends to provide knowledge regarding different components of coatings, the coating technologies including waterborne coatings, non-stick coatings, smart coatings etc.

Course objectives:

- To provide theoretical basis of the process of coatings and characteristics of coatings
- To make the students aware of the different essential components of paints and coatings
- To introduce to the different kinds of natural and synthetic resins and their applications
- To make the students familiar with the basic and recent advancements in coating technologies

Course outcome:

- Students will be able to appreciate the economical and societal importance of paints and coatings.
- They will be familiar with the components used in paints and will be able to predict the properties with varying compositions of the components.
- They will get knowledge about the manufacturing techniques for paints and coatings and the advancements in coating technologies.

Syllabus:

Introduction-concepts & terminologies, Concept of Dyes & Pigments driers, additives, solvents, plasticizers, Chemistry and Technology of resins-Natural & synthetic, processing techniques, properties, manufacturing of paints & applications of resins for surface coatings. Coil Coating, UV cured coating, Waterborne PU Coatings, Non Stick coatings, Smart Coatings, Hygienic Coatings, protective coatings, marine coatings, automotive and aerospace coatings, Characteristics and characterization of surface coatings

Detailed Version

Introduction: Concepts & terminologies, Interfacial tension, Free energy changes, wetting, dispersion, adhesion, Chemistry & Technology of Surfactants

Concept of Dyes & Pigments: Theory of Color; Important Physico-Chemical Characteristics of Pigments, Analysis & testing of pigments Inorganic Pigments; Chemistry, Properties and Applications of carbon black, metallic and metal oxide pigments, Resinated pigments, Organic Pigments, High Performance Pigments & Special effect pigments (IR Reflective, anticorrosive, thermo chromic, pearlescent etc), driers, additives, solvents, plasticizers.

Chemistry and Technology of resins: Natural resins like rosin, shellac, Bitumen, Asphalts and Coal tar – Their modifications & uses Chemistry and Technology of Synthetic resins viz. Alkyds, Polyester, Phenolics, Amino, Acrylic & Vinyl resins: Raw materials for these resins, Chemistry of synthesis of these resins, processing techniques, properties & applications of these resins for surface coatings.

Manufacture of paints & powder coatings: Powder Coatings, dry distempers, cement paints, oil based distempers and paints, other stiff paints, putties. marking and labeling of packaged products, Solvent emission, recovery and disposal, environmental, health and safety issues

Various surface coatings: Preparation and characteristics of Coil Coating, UV cured coating, Waterborne PU Coatings, Non Stick coatings, Smart Coatings, super hydrophobic coatings, electrowetting, Hygienic Coatings, protective coatings, marine coatings, automotive and aerospace coatings

Study of important characteristics of surface coating: Rheological properties, Optical Properties, Adhesion and Mechanical properties, Corrosion and Chemical resisting properties, Film thickness, Liquid Paint analysis according to ASTM, BIS and BS Standards, Characterization of Varnishes according to ASTM, BIS and BSS Standards

Books:

1. Arthur A. Tracton(Ed.), *Coatings Technology Handbook*, CRC press, 2006
2. Werner Freitag, Dieter Stoye (ed.), *Paints, Coatings and Solvents*, 2nd edition, Wiley-VCH, 2008.
3. Güngör Gündüz, *Chemistry, Materials, and Properties of Surface Coatings: Traditional and evolving technologies*. DEStech Publications, Inc., 2016.

4. Philip A. Schweitzer, P.E., *Paint and Coatings: Applications and Corrosion Resistance*, Taylor & Francis group, 2005.
5. Swaraj Paul, *Surface coatings: Science & Technology*, Wiley, 1996
6. R Lambourne, T A Strivens (Ed.) *Paint and Surface Coatings: Theory and Practice*, 2nd Edition, Woodhead publishing ltd, 1999.

CHM868

Advanced Characterization Techniques

Course Description:

Some of the important methods for materials characterization techniques are discussed in detail in this course. Students will learn about surface characterization, microstructural analysis, and elucidation of chemical composition and analysis of bandgap materials. Real-world examples of materials characterization will be discussed, including characterization of thin films, surfaces, interfaces, crystals and energy materials.

Course Objectives:

- To introduce some of the advanced characterization techniques aiding the cutting edge research
- Give hands-on training on available instruments (AFM, MS, CV)
- To provide in-depth knowledge in instrumental parameters and instrumentation
- To provide exposure in some frontier areas of the application

Course Outcomes:

- Students will learn to characterize materials to probe its structure & properties
- Students will understand how the materials will behave in technological applications with respect to its structural features.

Syllabus

X-ray diffraction (XRD); Indexing of XRD patterns, lattice parameter determination, determination of particle size and micro/macro strains. Surface mass spectrometry and mass spec imaging- MALDI, ESI, SIMS; Atom probe tomography; Cryoelectron microscopy; Cyclic voltammetry, electrochemical Impedance spectroscopy, Contact angle measurement, Surface area analysis, Dynamic Light Scattering, Nanoindentation,

Detailed version

- **X-ray techniques:** X-ray diffraction- Generation and characteristics of x-ray, Lattice planes and Bragg's law, Theory of diffraction, Wide angle XRD; determination of particle size and micro/macro strains.
- **Mass spectrometry in materials science:** Applications of Matrix assisted laser desorption ionization (MALDI) and electrospray ionization (ESI) in materials science. Surface imaging using mass spectrometry.
- **Atom probe tomography (APT):** field ion microscopy, instrumentation, local electrode atom probe, specimen preparation
- **Cryoelectron microscopy (CryoEM):** sample preparation, Image formation, Single particle cryo-EM, in situ cryo-EM

- **Electrochemical & Surface characterization techniques:** Cyclic voltammetry, Electrochemical Impedance spectroscopy, Contact angle measurement, Surface area analysis: Theory , experiment and its applications
- **Nanomaterial characterization:** using Dynamic Light Scattering, Introduction to particle size characterization, Dynamic Light Scattering: Particle size analysis, Zeta potential measurement: Instrumentation, basics and principle of analysis, Laser Doppler Electrophoresis: Stability of colloids, Elastic and plastic deformation-mechanical properties of materials, Nano indentation load-displacement curves, data analysis methods-Hardness testing of thin films and coatings.

Books:

1. Y. Leng, *Materials Characterization: Introduction to Microscopic and Spectroscopic Methods*, John Wiley & Sons, 2008.
2. J.C. Vickerman, I. Gilmore, *Surface Analysis: The Principal Techniques*, 2nd ed., John Wiley & Sons, Inc.2009.
3. H. Bubert, H. Jenett, *Surface and Thin Film Analysis: A Compendium of Principles, Instrumentation, and Applications*, Wiley-VCH, 2002.
4. S. Zhang, L. Li, A. Kumar, *Materials Characterization Techniques*, CRC Press, 2008.
5. Waseda, Yoshio, *X-ray diffraction crystallography introduction, examples and solved problems*, Springer-Verlag 2011
6. M. K. Miller , R. G. Forbes, *Atom-Probe Tomography:The Local Electrode Atom Probe*, Springer 2014
7. B. L. Nannenga, T. Gonen, *CryoEM Methods and Protocols*, Springer 2020.
8. Compton G. Richard and Craig E. Banks, *Understanding Voltammetry (2nd Edition)*, World Scientific, 2011.
9. Kock-Yee Law, Hong Zhao, *Surface Wetting Characterization, Contact Angle, and Fundamentals* Springer 2015.
10. S. Lowell, Joan E. Shields, *Powder Surface Area and Porosity* Springer 2013.
11. ASM Handbook: Materials Characterization, ASM International, 2008.
12. Mohan Ranganathan, *Materials Characterisation: modern methods and applications*; Pan Stanford 2015 ISBN: 9789814613064
13. S Zhang *Thin Films and Coatings: Toughening and Toughness Characterisation* CRC Press 2015,
14. Bruce J. Berne, Robert Pecora, *Dynamic Light Scattering: With Applications to Chemistry, Biology, and Physics* Dover Publications Inc.2003
15. Kenneth Schmitz, *An introduction to dynamic light scattering by macromolecules* Elsevier 2012.

Course Description:

This course emphasizes on the fundamental principles and materials science relevant to corrosion of materials. Mechanisms of different forms of corrosion (localised and environmentally assisted degradation), evaluation and methods of mitigation of corrosion, corrosion of materials used in industries, automobiles, vessels and aerospace sector are discussed.

Course Objectives:

- To introduce thermodynamic and kinetic aspects of electrochemical processes.
- To enable the students to understand the methodologies for predicting, measuring, and analyzing corrosion performance of materials.
- To provide hands on experience of operating potentiostatic equipment to conduct investigations on corrosion.
- To enable the students to identify methods for the prevention and remediation of corrosion.

Course Outcomes:

- The students will understand the causes and mechanisms of different forms of corrosion
- Students will get knowledge on the impact of composition, type of the material and its microstructure on corrosion.
- Students will be able to identify and propose materials with better corrosion resistance in specific environments.
- Students will be able to propose remediation to eliminate/reduce corrosion for a given material.

Syllabus

Corrosion definition, Electrochemical and thermodynamic principles, Pourbaix diagram, Corrosion rate expressions, Tafel equation, Passivity, Mixed potential theory, Forms of corrosion in metals & non-metals, Evaluation of corrosion & degradation of materials, Methods of corrosion prevention, Case studies.

Detailed Version

Introduction and basic concepts: Corrosion definition - Electrochemical and thermodynamic principles, electrode potential of metals, EMF and galvanic series, Faraday's laws Pourbaix diagram and its importance to iron, aluminium and magnesium metals

Electrochemical Kinetics of corrosion: corrosion rate expressions. Exchange current density, polarization - concentration, activation and resistance, Tafel equation, passivity, electrochemical behaviour of active-passive metals, factors governing metals exhibiting passivity, mixed potential theory and its application.

Forms of Corrosion: Atmospheric, galvanic, crevice, pitting, stress corrosion cracking, intergranular corrosion, corrosion fatigue, hydrogen damage, cavitation, fretting corrosion and high temperature oxidation-description, causes and remedial measures.

Corrosion measurement & testing : Purpose of testing, laboratory, semi-plant and field tests, susceptibility tests of IGC, stress corrosion cracking and pitting, ASTM standards for corrosion testing; polarization methods to measure corrosion rate, surface characterisation techniques.

Corrosion prevention : Corrosion prevention by design improvements, material selection, anodic and cathodic protection, metallic, non-metallic and inorganic coatings, mechanical and chemical methods and various corrosion inhibitors

Corrosion in industries: Corrosion in fossil fuel & power plants, automotive industry, aerospace industry, chemical processing industries, corrosion in petroleum production operations and refining, corrosion of pipelines. Corrosion in launch vehicles, related materials, launch facilities and in space environments.

Books:

1. D. A. Jones, *Principles and Prevention of Corrosion*, 2nd edition, Prentice Hall, USA, 1996.
2. H. H. Uhlig and R. W. Revie, *Corrosion and corrosion control : An introduction to Corrosion science and engineering* (4th ed.), John Wiley & Sons, 2008.
3. Fontana, M.G., Greene, N.D., *Corrosion Engineering*, 2nd edition, McGraw-Hill, USA, 1983
4. Philip A. Schweitzer, *Fundamentals of corrosion: mechanisms, causes, and preventative methods*, CRC Press, 2010

References:

1. Robert Baboian, *Corrosion Tests & Standards: Application & interpretation*, ASTM International, 2010.
2. Michael Dornbusch, *Corrosion analysis*, CRC Press, 2019.

CHM870

Thermodynamics and Phase Transformations in Materials

Objective

- To understand the rudiments of phase transformations through thermodynamics of materials for modelling of materials and alloy design
- To understand the concepts on phase stability and to explore the use of phase diagram for understanding various types of phase transformations that are relevant to metals and alloys

Learning Outcomes

- Construction of multicomponent phase diagrams using computational thermodynamic approach.
- Understand the variation of properties associated with the microstructural evolution during phase transformations

Course Content

Thermodynamics basic concepts: the first law, (the enthalpy concept, heat capacity), the second law (reversible and irreversible processes, entropy, Gibbs energy, chemical potential, driving force), the third law, Clausius-Clapeyrons equations.

Basics of Phase diagrams: Gibbs free energy – composition diagrams, Gibbs phase rule. Ideal and regular solutions, Diffusion: steady vs non-steady states, driving force and mechanisms

Interfaces: solid-vapour, grain and phase boundaries. Nucleation (homogeneous and heterogeneous), growth, Eutectic solidification

Solid state transformations: Recovery, recrystallization and grain growth. Eutectoid transformations, Order-disorder transformations, spinodal, and massive transformations. Transformations in steels and aerospace alloys

Reference books

- Introduction to the Thermodynamics of Materials, David R. Gaskell, 5th ed., CRC Press, 2008

- Raghavan, V., Solid State Phase Transformations, 1st edition, Prentice Hall India, 1987.
- Porter, D.A., Easterling, K. E., and Sherif, M.Y., Phase Transformation in Metals and Alloys, 3rd edition, CRC Press, 2009.
- Abbaschian, R., Abbaschian, L., and Reed-Hill, R. E., Physical Metallurgy Principles, 4th edition, Cengage Learning, 2009

CHM872

Fundamentals of Polymer Science

Course Description:

Polymers are one of the most important classes of materials. The curriculum of the programme comprises advanced courses concerned with polymeric materials, composites and applications. The course 'Fundamentals of Polymer Science' is intended to give thorough understanding about polymers and their properties to those students who did not study polymer science during their undergraduate courses. The course contents include basic concepts, polymerization mechanisms, kinetics, synthesis, thermal and mechanical properties and characterizations.

Course objectives:

- To provide knowledge in the basic concepts of polymer science
- To make the students familiar with the characterization techniques
- To make them aware the structure property relations of polymers

Course outcome:

- Students will understand and appreciate the importance of the polymers as an important class of materials
- Students will be well equipped to study the advanced courses related to polymer science and technology included in the curriculum

Syllabus:

Basic concepts, General mechanisms of polymerization reactions- synthesis, kinetics, techniques, Structure- property relationships of polymers. Copolymerization-mechanism-kinetics. Thermodynamics of polymer solutions, Crystal morphologies-Thermal transitions in polymers--Characterization and Testing- Molecular weight determination- Spectroscopy techniques, Thermal properties. Polymer degradation. Production, properties and applications of industrial polymers and general purpose rubbers. Applications of polymers in materials processing (ceramic, semiconductors and metals).

Detailed version

Basic concepts - Molecular forces - chemical bonding - Molecular weight studies - molecular weight distribution-configuration-conformation-Tacticity-Transitions in polymers-viscoelasticity-types of macromolecules-classification of polymers.

Structure and property relationships: Crystalline nature of polymers, factors affecting crystallization, crystallization and melting, melting: factors affecting. The glassy state and glass transition.

Mechanistic aspects: General characteristics of chain growth polymerisation, initiators, generation of initiators, free radical, anionic and cationic polymerization, ring opening polymerization, General characteristics of step growth polymerization, mechanism of step growth polymerization, coordination

polymerization. Kinetics of addition, condensation and coordination polymerization. Copolymerization mechanism, kinetics.

Polymerization techniques: Homogeneous polymerization techniques- Bulk, Solution, Heterogeneous polymerization techniques- Emulsion, Suspension, solid phase polymerisation.

Polymer solutions: Thermodynamics of polymer solutions, Solution properties of polymers, Solubility parameter, Conformation of polymer chains in polymer solutions, Flory-Huggins theory, Flory-Krigbaum theory, Solution viscosity, Osmotic pressure, Molecular size and molecular weight.

Characterization: End group analysis, colligative property measurement, ultra centrifugation, light scattering, gel permeation chromatography, Viscosity methods, IR, NMR etc. Thermal characterization,

Mechanical properties: Tensile, flexural, compressive, abrasion, endurance, fatigue, hardness, tear, resilience, impact, toughness.

Polymer degradation : Types of degradation: Thermal, mechanical, ultrasonic and photodegradation, oxidative and hydrolytic degradation, Biodegradable polymers

Industrial Polymers: Production, properties and applications of industrial polymers; PP, PE, PVC, PS, polyamide, polyacrylates, polyester (PET, PBT). General purpose rubbers: NR, SBR, NPR, EPDM etc.

Books:

1. F. W. Billmeyer, *Textbook of polymer science*, 3rd ed., John Wiley & Sons, Asia, New Delhi, 1994.
2. G. Odian, *Principles of Polymerization*, 4th ed., Wiley-Interscience, 2004
3. R. J Young and P. A. Lovell, *Introduction to Polymers*, 2nd ed., 2004

References:

1. M. Rubinstein, R.H. Colby, *Polymer Physics*, Oxford University Press, 2003.
2. P. Gosh, *Polymer Science and Technology*, Mc-Graw Hill, 2002.

CHM873

Specialty Polymers

Course description:

The course deals with recent developments in the field of synthesis of polymers which enable controlled synthesis of polymers for special applications. The course also gives an overview of polymeric materials used in electrical, electronic, optical and structural applications. The basic mechanisms and properties which enable polymers for applications in these fields and the synthesis, properties and applications of these specialty polymers are included.

Course objectives:

- To introduce the recent advancements in polymer synthesis
- To make the students aware that polymers have various applications based on their electric, electronic and optical properties.
- To make the students understand the mechanisms which enable the applications in these fields.

Course outcome:

- Students will be familiarized with the recent advancements in the field of polymer synthesis.
- They will be encouraged to explore these advanced techniques for synthesis of polymers with specified properties.
- Students will be aware of the potential of polymers in electric, electronic, optical and structural applications and will be ready to take up challenges to modify or synthesize polymers for these special applications.

Syllabus:

Specialty synthesis-ring opening polymerization, metathesis polymerization, ATRP, RAFT; heteroatomic polymers; electrically active polymers-conducting polymers, piezoelectric, pyroelectric and ferroelectric polymers, polymers for FET, electrical and electronic applications; photoactive polymers- photoresists, light emitting polymers, non-linear optical properties; ionic polymers- ionomers, polyelectrolytes; magnetically active polymers; Shape memory polymers; high performance polymers-polymer concrete, high modulus fibers, polymer explosives.

Detailed Syllabus

Polymer synthesis: General features of cyclopolymerisation, Ring-opening polymerization, Ziegler-Natta and metallocene catalysts. Metathesis polymerisation - mechanism of polymerization, Ring -Opening - Metathesis -Polymerisation (ROMP). Living polymerization by atom -transfer-radical-polymerization (ATRP), Reversible Addition Fragmentation Chain Transfer (RAFT), Speciality polymers like heteromatic polymers- poly ether ketones, polyphenylene oxide, polyphenylenesulphide, polysulphones, polysiloxanes, liquid crystalline polymers.

Electrically active polymers: Conjugated polymers, intrinsically conductive polymers, Polymers with piezoelectric, pyroelectric and ferroelectric properties, polymers used as insulators, polymers used in telecommunications, power transmissions etc. Polymers used for field emission transistors (FET), antistatic coatings, conducting adhesives, artificial nerves etc Electronic applications- EMI shielding, Frequency selective surfaces, satellite communication links

Photoactive polymers: Photo conducting polymers, polymers used in optical applications, photo resists and semiconductor fabrication, Light emission in polymers, Semi conducting materials as light emitting materials, Polymeric materials for second order nonlinear optical properties, photorefractive polymers, Polymers with high two photon activities.

Ionic Polymers: Ionic polymers (ionomers)-ionomers based on polyethylene, PTFE, polystyrene; Elastomeric ionomers; Polyelectrolytes - Characterization of polyelectrolytes, Application of polyelectrolyte complexes

Magnetically active polymers: Origin of magnetism in polymers, Iron, nickel, cobalt, ruthenium, osmium containing magnetic polymers, magnetic polymers with conductivity.

Shape memory polymers: Properties & applications

High performance polymers: Polymer concrete, Ultra high modulus fibers, polymer binders for propellants, Polymer explosives

Books:

1. Robert William Dyson, *Speciality Polymers*, 2nded., Blackie Academic & Professional, 1998
2. Manas Chanda, Salil K. Roy, *Industrial Polymers, Specialty Polymers, and their Applications*, CRC Press, 2008
3. Faiz Mohammad, *Specialty Polymers: Materials and Applications*, I.K. International Pvt Ltd, 2008

References:

1. Fried Joel R., *Polymer Science and Technology*, Prentice-Hall; 2nded. 2005
2. Johannes Karl Fink, *Hand book of Engineering and Specialty Polymers*, John Wiley & Sons, Vol.2, 2011
3. Norio Ise, Iwao Tabushi, *An Introduction to Speciality Polymers*, Cambridge University Press, 1983

Course Description:

Products made out of Natural and synthetic rubber finds innumerable domestic and industrial applications. This course is intended to provide knowledge on different kinds of rubbers, properties and manufacturing of useful articles from rubbers. The course discusses the theory on rubber elasticity, compounding, curing, moulding technologies and testing.

Course objectives:

1. To provide knowledge on different kinds of rubbers and their properties.
2. To make the students familiar with compounding, curing and moulding technologies for different kinds of rubber
3. To make the students capable of selecting and designing the suitable rubber for specific applications

Course Outcome:

1. Students will appreciate the immense developments in materials science with advancements in rubber technology
2. Students will be familiarized with the processing of rubber and manufacturing of products
3. They will be able to judiciously select and analyse the appropriate testing method for specific rubber products.

Syllabus:

Introduction to Rubbers and elastomers; Manufacture, structure, properties and applications of Natural Rubber, Synthetic rubbers like SBR, Butyl rubber, EPDM, Hypalon, nitrile rubber etc; Chemistry and technology of rubber vulcanization; Rubber compounding, additives used in rubber compounding; General compound design, kinetics of vulcanization; Assessment of curing; Compression, transfer, extrusion, calendering and injection moulding of rubbers; Manufacturing, testing and recycling of rubber products.

Detailed Version

Introduction to Rubbers and elastomers: Elastic nature, Basic theory of rubber elasticity, Elasticity of single molecule and three dimensional network etc

Natural rubber and synthetic rubbers: Manufacture, structure, properties and applications of Polyisoprenes, styrene butadiene rubber, Butyl rubber, EPDM, Hypalon, silicones, butyl rubber and halobutyl rubber, nitrile rubber, thermoplastics elastomers, latex and foam rubber.

Compounding of Rubbers: Chemistry and technology of rubber vulcanization, mastication, rubber compounding, additives used in rubber compounding: Vulcanizates, Fillers - reinforcing and non-black fillers, plasticizers, peptizers, accelerators, activators, softeners, anti-aging additives, colorants, flame retarders, blowing agents, deodorants, abrasive, retarders etc.. Machineries used for mixing- Mixing mills, internal mixers, banbury mixers etc

Curing process of rubber compounds: General compound design, kinetics of vulcanization, chemical reactions, factors affecting rate of vulcanization etc. Assessment of curing -Viscometers, Capillary Rheometers, Rotational Rheometers and plastometers.

Moulding Technology: Compression, transfer, extrusion, calendering and injection moulding of rubbers. Manufacturing technology: Manufacturing of products such as tyres, tubes, conveyor belts and flat belts, cellular products, hose technology, cables, footwear and latex goods, rubbers used in power transmission, O-rings, gaskets and seals

Testing of raw rubbers, compounds and rubber products, Recycling of rubber products

Books:

1. Maurice Morton, *Rubber Technology*, Academic Publishers, 2010
2. C M Blow, *Rubber Technology and Manufacture*, Butterworth-Heinmann, 2nd Edition, 1982.
3. Werner Hoffmann, *Rubber Technology Handbook*, HANSER Publishers, 1989

References:

1. Bredan Rodgers, *Rubber Compounding Chemistry and Application*, CRC Press; 1st ed. 2004
2. G. S. Whitby, *Synthetic Rubber*, Wiley, New York, 1954
3. John S. Dick, R. A. Annicelli, *Rubber Technology: Compounding and Testing for Performance*, Hanser Publishers, 2001

CHM875

Smart and Intelligent Materials

Course Description:

Smart materials can sense and respond to the environment in optimal manner and hence gains much significance in new materials technologies for achieving energy security, effective healthcare and food security to support sustainable cities in the near future. The course is intended to provide an overview of different classes and categories of smart materials and their synchronous roles in building smart systems. The effective application of any material being dependent on the ability to tailor its properties, various mechanisms governing the smart behavior in smart alloys, smart polymers, piezoelectric materials and chromogenic materials are discussed. The wide range of applications of smart materials with emphasis on space applications is also included.

Course objectives:

- To introduce students to various classes of stimuli responsive materials
- To develop molecular/atomic level understanding of the smart behavior in the materials
- To signify the huge potential/crucial role of smart materials/systems in the future technology development

Course outcome:

- Students will get introduced to ‘intelligence’ and smart behavior in materials
- The vast potential of smart materials will encourage students to explore them in detail and to design them for specific applications
- The course would also enable the students to appreciate the huge role of bio inspiration in the design of next generation materials

Syllabus:

Smart materials and structures- piezoelectric materials, piezoceramics, piezopolymers; Shape memory materials- one way and two ways SME, Training of SMAs, Functional properties of SMAs; Chromogenic materials- principles and design strategies; Smart polymers- temperature responsive and light responsive polymers, Molecular imprinting using smart polymers, Smart hydrogels, Fast responsive hydrogels, Applications; Smart systems for space applications- smart corrosion protection coatings, Self-healing materials, Sensors, Actuators, Deployment devices

Detailed version

Smart materials and structures: System intelligence- components and classification of smart structures, common smart materials and associated stimulus-response, Application areas of smart systems

Categories of smart materials: Ferroelectric materials: Piezoelectric materials- piezoelectric effect, Direct and converse, parameter definitions, Piezoceramics, Piezopolymers, Piezoelectric materials as sensors, Actuators and bimorphs

Shape memory materials: Shape memory alloys (SMAs), Shape memory effect, Martensitic transformation, One way and two-way SME, training of SMAs, binary and ternary alloy systems, Functional properties of SMAs

Smart polymers: Shape memory polymers - heat, light and electro actuations. Synthesis of shape memory polymers, Bioinspired systems, Protein-based smart polymers, pH-responsive and photo-responsive polymers, Self-assembly, Molecular imprinting using smart polymers, biomedical applications of smart polymers.

Chromogenic materials: Thermochromism, Photochromism, Electrochromism, Halochromism, Solvatochromism- principle and design strategies with examples from each category

Smart hydrogels: Synthesis, Fast responsive hydrogels, Molecular recognition, Smart hydrogels as actuators, Controlled drug release, Artificial muscles, Hydrogels in microfluidics

Smart systems for space applications: Elastic memory composites, Smart corrosion protection coatings, Self-healing materials, Sensors, Actuators, Transducers, MEMS, Deployment devices, Molecular machines

Smart Materials in Additive Manufacturing: Principles for 4D printing - - origami-inspired 4D printing, 4D microprinting, reversible 4D printing and 4D bioprinting - modeling and fabrication of 4D printed materials - dielectric elastomer soft robots, low-voltage electroactive polymers, and stimuli-responsive hydrogels. 4D printing of light-responsive structures, gels and soft materials, and natural fibre composites and related applications.

Text Books

1. M. Schwartz, New Materials, Processes, and Methods Technology, CRC Press, 2006.
2. K. Otsuka, C.M. Wayman (Eds.), Shape Memory Materials, Cambridge University Press, 1998.
3. Smart Materials in Additive Manufacturing, volume 1: 4D Printing Principles and Fabrication 1st Edition - June 25, 2022. Editors: Mahdi Bodaghi, Ali Zolfagharian; Paperback ISBN: 9780128240823 eBook ISBN: 9780128240830
4. M.V. Gandhi, B. S. Thompson, Smart Materials and Structures, Chapman & Hall, 1992.

References

1. D.J. Leo, Engineering Analysis of Smart Material Systems, Wiley 2007.
2. P. Ball, Made to Measure: Materials for the 21st Century, Princeton University Press, 1997.
3. I. Galaev, B. Mattiasson (Eds.), Smart Polymers: Applications in Biotechnology and Biomedicine, 2nd ed., CRC Press, 2008.
4. N. Yui, R. J. Mersy, K. Park (Eds.), Reflexive Polymers and Hydrogels: Understanding and Designing Fast Responsive Polymeric Systems, CRC Press, 2004.
5. Smart Materials Taxonomy, Victor Goldade, Serge Shil'ko, Aleksander Neverov; CRC Press, Taylor and Francis, 2015
6. M. Addington, D.L. Schodek, Smart Materials and New Technologies in Architecture, Elsevier 2005.
7. Smart Materials in Additive Manufacturing, volume 2: 4D Printing Mechanics, Modeling, and Advanced Engineering Applications 1st Edition - June 25, 2022 Editors: Mahdi Bodaghi, Ali Zolfagharian Paperback ISBN: 9780323954303 eBook ISBN: 9780323954310

Course Description:

This course will focus on the fundamental principles required to understand various battery technologies. The course gives an overview of primary and secondary batteries (lead –acid, Ni-MH, Li-ion and metal – air etc), supercapacitors and fuel cells. Their manufacturing, fabrication, operation, performance and safety are also included. In nut shell, the course discusses the design and development of modern electrochemical energy systems.

Course Objectives:

- To provide the basic physical concepts required to understand energy storage technology
- To help the students to explore the materials used in various components of electrochemical energy systems
- To discuss the performance characteristics and characterization methods of battery/supercapacitors/fuel cells
- To provide hands on experience on fabrication and testing of battery/supercapacitors (coin cell level)
- To explore the processes of production and applications of electrochemical energy storage systems.

Course Outcomes:

- The students will understand the materials, fabrication, operation and analysis of electrochemical energy storage systems
- They will acquire the ability to design and develop materials for energy storage systems.
- They will be able to appreciate the complete picture of electrochemical energy storage technology.

Syllabus:

Basic concepts, Primary and Secondary cells, Materials for batteries, supercapacitors and fuel cells, Electrochemical energy storage systems, Design, fabrication, operation and Evaluation; Safety and tolerance

Detailed version

Basic concepts: Reversible cells and irreversible cell reactions, Parameters for characterizing batteries

Batteries: Primary and Secondary cells, Chemistry and materials used for various components (electrodes, electrolytes, separator and binders) of different types of batteries: Leclanche/Dry/Alkaline cell, Silver cell, Mercury cell, Lead-acid battery: safety and design; Edison Cell, Ni-Cd battery, Ni Metal Hydride (Ni-MH) battery, Ni-Hydrogen battery, Sodium-Sulfur battery, Lithium-ion/Lithium-polymer/ Li-S battery, Metal-air batteries and their applications

Performance & Manufacturing of batteries: Charge-Discharge characteristics, Energy/power density, overcharging, Mechanics of battery cells and materials, Manufacturing of batteries. Battery safety and Abuse tolerance, Coupling with other energy storage devices.

Super/ultracapacitors: Fundamentals of Electrochemical Supercapacitors, Electrode and electrolyte interfaces and their capacitances, Charge-Discharge characteristics, Energy/power density, Design, Fabrication, operation and evaluation, Thermal management; Supercapacitor stack manufacturing and construction, Coupling with batteries and fuel cells; Applications

Fuel cells: Overview of key fuel cell technologies- various types of fuel cells, materials for electrodes, electrolytes and other components, working mechanisms, hydrogen generation and storage; limitations, recent progress in fuel cells.

Books:

1. A.J. Bard, L.R. Faulkner, *Electrochemical Methods, Fundamentals and Application*. Wiley, 2001.
2. C. Daniel and Jurgen O. Besenhard, *Handbook of Battery Materials*, Wiley-VCH Verlag, 2011
3. K.E. Aifantis, S.A. Hackney, and R. V. Kumar (Ed.) *High Energy Density Lithium Batteries Materials, Engineering, Applications*, Wiley-VCH Verlag GmbH & Co. KGaA, 2010.
4. A.Yu, V. Chabot, and J. Zhang, *Electrochemical Supercapacitors for Energy Storage and Delivery Fundamentals and Applications*, Taylor & Francis Group, 2013.
5. F. Beguin and E. Frackowiak, *Supercapacitors- Materials, Systems, and Applications*. Wiley-VCH Verlag GmbH & Co. 2013.
6. V. Hacker, S. Mitsushima(Eds.) *Fuel Cells and Hydrogen: From Fundamentals to Applied Research*, Elsevier, 2018

CHM878

Materials and Technologies for Sustainable Energy

Course Description

Renewable energies are the future energy sources. Armed with feasible and commercially viable technologies they can provide major solutions for a sustainable energy future. Though the resources are available in plenty, the cost of conversion is high even for the matured technologies mainly because of the lack of wide usage and vice versa. Thus, understanding of the available sources, their significance and the conversion technologies by the students is crucial at this juncture. The course addresses the above mentioned issues and provides understanding of the various renewable sources and the technologies which are available with emphasis on materials and the mechanism.

Objectives:

- To introduce the student to the environmental impacts of current energy utilization and the importance of switching to the renewable energy sources for a sustainable future
- To provide the students with the knowledge of available materials and technologies for tapping the renewable energy resources
- To impart understanding of the underlying mechanism of the different sustainable technologies
- To develop skills to contributing to the advancement of sustainable energy solutions

Outcome:

- The students will understand the environmental impacts of conventional energy sources and the importance of switching to renewable energy sources for future energy needs.
- Students will gain knowledge on various renewable energy sources, their potential, and the different methods used for energy conversion methods.
- Students will learn about the functioning and technological advancements of solar cells, fuel cells, different generations of solar cells, and other renewable technologies such as photocatalysis and the hydrogen economy.

- Students will analyze the characteristics and mechanisms of materials used in renewable energy technologies, enabling selection of materials for sustainable energy solutions.
- Students will evaluate the performance of different renewable energy technologies and materials, considering their efficiency, cost, and sustainability.
- Students will apply knowledge of renewable energy materials and technologies to propose or identify new materials and technologies for green energy applications.
- Graduate develop skills to modify existing materials or technologies for enhanced performance in renewable energy applications, contributing to the advancement of sustainable energy solutions.

Syllabus:

Global Energy Demand, Renewable Energy Sources, Materials & Technologies. -Solar Energy, Photovoltaic cells, Photocatalysis Photoelectrochemical cells. Mechanism, Fabrication, Evaluation, and Efficiency. Future energy economy-Hydrogen economy- Fuel cells.

Detailed Version

Introduction: Global Energy Demand and Use, Impacts of conventional energy utilization, Renewable Energy Sources- Hydroelectric, Wind, geothermal and Tidal Energy –Conversion, potential and limitations–Economical and Environmental Aspects of conventional and renewable energy systems and the need to switch to low emission or zero emission methods.

Solar Energy and Solar Cells: Solar Spectrum, Solar constant, Passive conversion –Materials for Renewable energy conversion- Photovoltaics --Silicon (Si) solar cells, Crystalline/ Semicrystalline/ Amorphous Si solar cells, Thin film solar cells. Organic solar cells- bilayer, Bulk heterojunction, polymer solar cells, perovskite based solar cells, hybrid solar cells. Efficiency; limiting factors.

Hydrogen production: Water splitting Photoelectrochemical cells - Photoelectrolysis, photochemical cells, photocatalysis, Mechanism- electron transfer: Factors affecting electron transfer.

Sustainable Energy Technologies: Fuel cells-, Various types, Materials- Fuels- Reforming, Electrodes, Catalyst, electrolyte -efficiency. Internal resistance, general causes for failure. Future energy economy- Hydrogen economy –Hydrogen storage: Materials and Processes

Books:

1. B.K. Hodge, *Alternate Energy Systems and Applications*, John Wiley & sons, Inc., 2010.
2. Alan J. Heeger, Niyazi Serdar Sariciftci and Ebinazar B. Namdas, *Semiconducting and Metallic Polymers*, Oxford Univ Press 2010.
3. W. Streicher and M. Kaltschmitt (Ed.) *Renewable energy. Technology, economics and environment*, Springer, 2007.
4. N. Armaroli, V. Balzani and N. Serpone, *Powering Planet Earth – Energy Solutions for the Future*, Wiley, 2012.

References:

1. C. Brabec, *Organic Photovoltaics*, Wiley-VCH, 2008.
2. Norman S. Allen (Ed.), *Photochemistry and Photophysics of Polymeric Materials*, 2010.
3. X. Moya David and Muñoz-Rojas(Ed.), *Materials for Sustainable Energy Applications Conversion, Storage, Transmission, and Consumption*, 2016, Pan Stanford Publishing Pvt. Ltd.
4. L. Liu and S. Bashir, *Advanced Nanomaterials and their Applications in Renewable Energy*, Elsevier Science, 2015.

Lab courses (4 Nos)

CHM631

Lab 1: Applied Mathematics and Process Modeling

Experiments:

To develop a model and solve for

1. Fully developed flow
2. Steady state heat conduction in large plate
3. Steady state two dimensional heat conduction
4. Transient state two dimensional heat conduction
5. Plug flow reactor
6. Batch reactor
7. CSTR in series with constant hold up
8. CSTR with feedback control
9. Numerical solution of ODE/PDE using MATLAB

CHM633

Lab2: Materials Synthesis and Characterization

Experiments:

1. Synthesis and characterization of nanomaterials
 - a. Sol-gel synthesis: TiO_2
 - b. Metallic nanoparticles: Ag@citrate and Au@citrate, Ag@borohydride, Ag@PVP
 - c. CdS quantum dots
 - d. Graphene by Hummer's method
 - e. Functionalisation of CNT's
2. Template based synthesis of nickel nanowires and characterization using optical & atomic force microscopy
3. Nanocomposite (nanoclay based systems& functionalized CNTs)
4. Evaluations of structure-property relationship in polymers: Analysis includes: molecular weight determination, viscosity, rheology, TGA, DMA and mechanical properties of at least four polymers
5. Determination of kinetics of spherulite growth using polarized optical microscope
6. Electrical conductivity measurement of polymers using electrochemical workstation
7. Diffusion and gas permeability measurement of polymer films
8. Powder synthesis: XRD characterisation, particle size, surface area analysis
9. Dependency of molecular weight of a polymer with different initiator concentration: establishment of square root law
10. Reactivity ratio of co-monomers: Fineman-Ross method
11. Kinetics of acid catalyzed poly esterification

CHM641

Lab 3: Composite and Processing

Experiments:

1. Preparation and characterisation of compression moulded random, bidirectional and unidirectional composites based on thermoplastic, thermoset and elastomer
2. Preparation and characterization of short fibre composites using vacuum bag, injection moulding, extrusion methods
3. Preparation of laminates
4. Determination of fiber-volume ratio
5. Determination of tensile properties of composite
6. Determination of compressive properties and shear properties of unidirectional lamina
7. Determination of interlaminar shear strength, interlaminar tensile strength, interlaminar fracture toughness.
8. Biaxial testing of laminates

CHM644 Lab 4: Aerospace Materials

Experiments:

1. Preparation of a high temperature thermal insulating foam and study its microstructure, thermal diffusivity / thermal conductivity
2. Heat treatment studies on super alloys and aluminium alloys to understand the precipitation hardening
3. Studies on shape memory effect on Nitinol
4. Compression tests on aerospace alloys and foams for thermal protection to evaluate the stress-strain behavior and their plastic constants
5. Single-shear and double shear testing on welded joints
6. TIG Welding of and its qualification using NDT technique such as Ultrasonic Testing/Radiographic testing and dye penetration testing
7. Electrochemical corrosion studies on aerospace alloys using Tafel plot method
8. Metallographic studies on forged and welded metals/alloys
 - (a) to analyze the grain flow pattern in forged samples
 - (b) Analyzing the weld zone, heat affected zone and parent metal of the welded sample
9. Aging studies on aluminium alloys using differential scanning calorimeter
10. Machinability studies on aerospace alloys
11. Measurement of flammability, flame penetration time and char yield of an ablative material
12. Preparation and characterization of a ceramic matrix composite
13. Effect of ball milling time on particle size and surface area of a ceramic/metal powder
14. Fabrication and evaluation of dye sensitized solar cell
15. Studies on charge-discharge characteristics of a battery

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